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A Complex-Geometry CFD Model for Chemical/Biological Contaminant Transport Problems

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Abstract

Today's world faces threats from unintended environmental disasters such as a railroad tank car derailment or a gas main break as well as the ever-present specter of terrorist action. In response to the threat posed by the proliferation of chemical and biological weapons worldwide, the Department of Defense requires a capability to compute the propagation of contaminants throughout geometrically complex environments under a variety of meteorological conditions. The FAST3D-CT code, an application of the Flux-Corrected Transport algorithm to contaminant transport problems, represents a current hazard assessment capability for urban environments. The model aims to support consequence management operations for chemical/biological incidents occurring in urban environments and/or complex terrain. High Performance Computing resources are being used to refine and calibrate this scalable Computational Fluid Dynamic model over a wide range of applications. The present study focuses on the detailed simulation and analysis of both hypothetical (proof-of-principle) and staged (live field trial) contaminant releases. Proof-of-principle demonstrations include external release scenarios involving two Washington, DC, landmarks, namely the Pentagon and its surroundings, and the DC Mall area. Live field demonstrations involve simulated contaminant releases within a generic apartment complex. For the live field trials investigated, direct connectivity between internal and external flow environments is a prerequisite to modeling accuracy.

Introduction

Environmental disaster readiness and counter-terrorist planning, as well as military training, campaign planning, and operations, make a sound Modeling and Simulation (M&S) capability as important to the civilian sector as to the military. Hazard prediction tools enable first responders to make timely, educated decisions regarding rescue and evacuation procedures. They can also be used as planning tools for the optimal use of federal, state, and city resources to mitigate a disaster involving the release of chemical or biological agents.

Current hazard prediction tools used by the Department of Defense (DoD) are generally limited to outdoor scenarios using limited terrain data. A clear need exists for models that can compute the flow and deposition of contaminant particles and gases within and around buildings of varying complexity under a variety of meteorological conditions. The Naval Research Laboratory has recently extended its scalable FAST3D Computational Fluid Dynamics (CFD) model to contaminant transport problems for urban and environmental hazard assessment. The suite of FAST3D software underlying the new contaminant transport (CT) version is being optimized for parallel computing under a project sponsored by the High Performance Computing (HPC) Modernization Program, namely the DoD Common HPC Software Support Initiative.

The application of detailed CFD models to chemical/biological (C/B) transport problems is relatively new and requires considerably more computer resources than traditional models. However, the gains are proportionally dramatic. The advantages include the ability to model complex geometry, to dynamically resolve flow field details, and to handle problems on the interface between regimes where neither zonal (indoor) nor Gaussian "puff" (outdoor) models are valid. Assumptions in CFD models are, in general, fewer and less restrictive than in zonal and Gaussian models.

The viability of using a detailed CFD model such as FAST3D-CT to support C/B consequence management was recently demonstrated during the 911-Bio Advanced Concept Technology Demonstration (ACTD). The ACTD leveraged existing M&S technology by applying select CFD and zonal airflow models to consequence management problems. Two different scenarios (i.e., simulated contaminant releases in two different facilities) were used in the 911-Bio ACTD. Participation in the live field trials led to the development of a FAST3D-CT software suite capable of providing a coupled interior/exterior modeling where flow circulation, leaks and the external wind field define effective contaminant transport.

This paper presents a status report on three related FAST3D-CT modeling initiatives currently underway that are being supported by an HPC Challenge Grant. Large-scale applications focus on external release scenarios about Washington's Pentagon and DC Mall areas, and internal release scenarios within the German Village apartment complex, Dugway Proving Ground, UT, a component of the 911-Bio ACTD. These and future computations are being used to further validate and calibrate the FAST3D-CT model, to establish a database for calibrating simpler models, to analyze a few important scenarios of immediate national and military concern, and to establish operational rules of thumb for counter-terrorism procedures and preparations at large, inhabited events.

Numerical Model

The time-dependent, numerical simulations were performed using FAST3D-CT, an extension of the FAST3D model (Young et al., 1993) to the particle and flow physics of contaminant transport problems. The model was designed from the beginning to be compatible with parallel computer architectures. The model's three-dimensional flow solver is based on the Flux-Corrected Transport (FCT) algorithm. FCT (Boris and Book, 1973; Boris et al., 1993) is a high-order, monotone, positivity-preserving method for solving generalized continuity equations with source terms. Monotonicity is achieved by introducing a diffusive flux and later correcting the calculated results with an antidiffusive flux modified by a flux limiter. Operator splitting techniques are used to divide the solution for the three-dimensional flow into a series of one-dimensional integrations along each coordinate direction.

Complex geometry capabilities are provided by the Virtual Cell Embedding (VCE) algorithms. VCE is a method for representing and computing the flow around bodies of arbitrary shape on a Cartesian grid without sacrificing computational speed or memory (Landsberg et al., 1994). Although the grid remains orthogonal, the VCE method effectively increases the number of mesh points in the vicinity of complex geometric shapes, thus eliminating "staircase" effects. If any cell is partially obstructed by an obstacle or wall, the flux calculation is modified by subdividing each of the partially blocked cells into a number of smaller subcells from which the areas and volumes may be computed to arbitrary accuracy. Only those cells next to the boundary are refined or subdivided. A flux coupling vector between the three integration directions is used in the direction-split integration of the flow solution to correct the apparent fluid compression in each cell caused by the obstructing body. The flux coupling term is computed and used as a source term in the FCT integration.

In its current form, the numerical model solves the time-dependent conservation equations for mass, momentum, and total energy. This set of equations is closed by including the perfect gas equation of state in the definition of the total energy. FAST3D-CT has an implicit Large Eddy Simulation (LES) turbulence model and the ability to track passive flow tracers, including gases and particles. Multi-species particle and gas phase contaminants can be initialized, sprayed or injected from localized sources, transported, and diagnosed in real time. However, these capabilities are, to date, invoked in a problem-by-problem manner. The model requires geometric and environmental input data to satisfy initial and boundary condition requirements for the computational domain. Time-varying meteorological conditions can be accommodated. The model can resolve complex, multi-compartment geometries that can be modified when seeking finer resolution or simulating new physical conditions, such as opening or shutting doors or windows.

Two of the fundamental software technology components in the FAST3D-CT model, the general flow solver FAST3D and the grid generator GRIDVCE, have been implemented on several scalable systems. An efficient running-transpose data structure is employed which helps preserve much of the original FCT code and its cache-oriented structure. A system of virtual nodes is incorporated to simplify the transpose on varying numbers of physical nodes, to permit a change in the number of actual physical nodes in mid-simulation, and to provide fault tolerance for the very long run times required. This allows simulations with very complex geometry to be initialized on more easily programmed serial computers and also allows the results to be analyzed off-line by sharing dump/restart files. About 25%-35% of theoretical peak efficiency is being obtained, depending on the complex geometry and actual HPC architecture. In addition, it has been shown that the time taken for FCT integrations and the other dynamic operations scale as the inverse of the number of nodes. On the Intel iPSC/860, the current FAST3D code has shown linear speed-up to 256 nodes. This is repeatedly confirmed on the IBM SP-2, Silicon Graphics 2000, and Convex Exemplar systems.

An MPI interface to vendor-specific message passing libraries has been implemented to handle the communications requirements and should accommodate most current platforms. Since geometrical feature data is packed and stored along with the flow field data, the native word sizes and formats are machine-specific. FAST3D algorithms have been written to be equally efficient on single processor and massively parallel distributed memory computers. The current version of FAST3D-CT runs with essentially no change on a wide range of systems; calculations can be started on one scalable system and finished on another.

Proof-of Principle Demonstrations

Pentagon and its Surroundings

In its first application, the FAST3D-CT model was used to simulate the propagation of a gas cloud over the Pentagon. This initial proof-of-principle demonstration was performed for the HPC Modernization Program using 1996 DoD Challenge Grant resources. Shown in Figure 1 is a series of snapshots that span the 40-minute period after the start of a continuous plume release just northwest of the building (i.e., upper left hand corner of the first snapshot). Nearby buildings and road embankments, as well as the Pentagon, affect the convection of the contaminant. This three-dimensional computation was performed on an Intel iPSC/860 using about 1.2 million grid points for 6-meter resolution.

An update to the original Pentagon simulation was recently completed using approximately the same number of grid points (1.2 million) to maintain 6-meter resolution. The computational domain of this latest simulation adds a power plant near the Pentagon, additional buildings in the Crystal City region, and a fractal-like representation of trees to the original domain. Figure 2 presents the same series of snapshots as did Figure 1. Comparing the two simulations reveals the substantial effect the trees have on the propagating cloud. The tree canopy effectively entraps some of the gas cloud while dispersing and retarding the portion that propagates downstream towards Crystal City. This new computation was completed in real time (i.e., in less that 40 minutes) using 8 processors of a SGI Origin 2000.

DC Mall Area

Several Challenge Project simulations over city areas such as Washington, DC, are planned to demonstrate the feasibility of using a scalable CFD model to simulate a chemical/biological release scenario in a high-density urban environment. These urban computations will incorporate the full geometry of the city, wind fields provided by mesoscale simulations and insitu measurements, and a recently demonstrated fractal model of trees enabled by the VCE algorithms.

Rapid and inexpensive digital specification of geometry and grid generation for urban areas and buildings has become a pacing item. In preparation for a series of building-block simulations involving the DC Mall area, an efficient VCE-tailored method of constructing city elements has been developed. This method is being used to construct a DC Mall database, a section of which is shown in Figure 3, from which computational grids of arbitrary resolution can be generated. The resulting database will define the complex array of buildings, streets, and other significant structures that comprise the DC Mall area as a function of elevation. A release scenario compatible with a building-block approach will be used so that the geometry can be easily refined to include more and more features in subsequent simulations.

Live Field Demonstrations

The FAST3D-CT model was used to perform detailed simulations of the 1997 Bacillus subtillis var. niger and propylene release trials conducted during the 911-Bio ACTD (Cybyk et al., 1999a, 1999b, 1999c). The primary ACTD experiments were staged at the Michael Army Airfield (MAA) hangar and the German Village (GV) apartment complex, Dugway Proving Ground, UT. "Reach back" (i.e., post-experiment) simulations of both geometries were performed using internal building measurements, heating, ventilation, and air conditioning (HVAC) system conditions, and external meteorological conditions at the time and location of the trials. Follow-on efforts to the on-line computations performed at the field trials have focused on model calibration and validation, and input sensitivity studies (Cybyk et al., 1999b). The following section discusses the most recent FAST3D-CT simulations performed of German Village release scenarios and compares the "blind" numerical predictions to experimental data.

German Village

The ACTD experiments conducted at the German Village complex involved propylene release trials that took place in the center apartment on the southern side of the building. Cross-sectional views of the apartment complex geometry, as represented by the numerical model, and sampler locations are shown in Figure 4. Time histories of propylene concentrations were collected during the trials at twelve locations in the apartment. Each sampler was located five feet off the floor in approximately the center of a given room. In addition, internal building measurements, HVAC performance characteristics, and external meteorological conditions were collected as part of the ACTD experiments for use as model inputs.

FAST3D-CT simulations were performed using building leakage characteristics, HVAC system conditions, and wind measurements provided by the experimentalists. Each simulation resolved individual rooms on all three floors of the apartment, including the apartment stairwell and HVAC system, using grid resolution of 0.25 meters in all three coordinate directions. Externally, the same 112 by 64 by 80 grid resolved other local structures that may affect the winds encountered by the subject apartment, such as the structure and rooflines of adjoining apartment units, allowing connection of the internal behavior of the contaminant to the time-dependent escape into the external environment. For the two GV scenarios shown in the Figure 5, the large leaks in the attic have a significant effect on interior flow patterns due to the strong external winds flowing over the building.

Time histories of propylene concentrations at several sampler locations as well as total propylene histories within the facility are shown in Figure 6 for the GV9 case. The 24-gram propylene release occurs over a three minute period in the simulation. As expected, the peak concentration in the release room (room 1.3) occurs at t = 3 minutes. Propylene levels in the other rooms begin to rise after approximately three minutes and do not peak until about a half hour into the simulation. Comparisons between measurements and blind predictions are encouraging, especially considering the influence facility leakage and HVAC performance characterizations and meteorological conditions can have on internal contaminant release modeling (Cybyk et al., 1999b). The effect of the leakage of the gas out of the building is seen in the bottom plot of Figure 6, where the total amount of propylene within the building is plotted against time. A small integration error in a FAST3D-CT diagnostic is believed to account for the rise in the total propylene in the building for the few minutes after completion of the release itself. However, this error should not effect the total propylene values after the curve peaks. The primary observation made in the simulation is that the large leaks in the attic have a significant effect on interior flow patterns. This effect is due to the spatially-varying pressure distributions along the attic wall exteriors set up by the strong external winds flowing over the building rooftop.

Future Thrusts

The primary objective of the NRL CT effort is to develop, calibrate, validate, and document FAST3D-CT as a hazard assessment model for operational C/B use. The effort targets a generic class of fluid dynamic applications characterized by slow, time-dependent, mostly incompressible flows resulting from the interaction of ambient winds with local topography and man-made structures. A secondary objective is to perform a documented set of simulations and sensitivity studies that serve three purposes: 1) to provide a reliable, high-resolution database for calibrating other models; 2) to analyze a few important scenarios whose characteristics are of immediate national and military concern; and 3) to extract rules of thumb from the simulations that are suitable for training Incidence Response Teams tasked with C/B consequence management.

With these long-term objectives in mind, efforts to date have focused on the development and testing of physical models, numerical algorithms, interfaces to meteorological models, and user interfaces necessary to extend the FAST3D software suite towards support of consequence management operations. Large-scale simulations have been used to demonstrate newly developed capabilities and to calibrate and validate the underlying models. Ongoing applications involve a nested set of grid convergence simulations based on the detailed measurements of the ACTD field trials. While calibration and validation efforts will continue indefinitely, future applications will involve sponsor-selected urban geometries that incorporate wind fields provided by mesoscale simulations and insitu measurements. It is this coupling to atmospheric data that will enable FAST3D-CT to provide a credible realization of the dispersion, transport, and deposition of contaminants in realistic geometry under evolving real atmospheric conditions.

Conclusions

Detailed contaminant transport modeling that includes the effects of realistic complex geometry is central to any technology aimed at providing a timely, effective response to a chemical or biological threat or to assess the effects of an obscurant cloud. The FAST3D-CT model represents a current hazard assessment capability for urban environments. This paper discusses numerical simulations of both hypothetical and staged C/B release scenarios performed using the FAST3D-CT CFD model.

Presented was a status report on three related modeling initiatives currently underway that are being supported by an HPC Challenge Grant. Completed and ongoing proof-of-principle demonstrations include external release scenarios involving two Washington, DC, landmarks, namely the Pentagon and its surroundings, and the DC Mall area. Continuing calibration and validation efforts center around the 911-Bio ACTD database, specifically internal release scenarios involving a generic apartment complex (German Village) and a convention center mockup (MAA hangar). Overall progress to date has demonstrated the feasibility of extending and applying an existing CFD model to consequence management problems in complex urban environments.

Although a critical "first step," further technology development is required to mature the software suite into a hazard assessment model for operational chemical/biological use. High Performance Computing resources are necessary to perform high-priority, sponsor-selected applications. Furthermore, HPC resources are necessary to adapt and calibrate a complimentary set of existing CT models to chemical/biological applications, to integrate them into a multi-media system, and to demonstrate the new capability under challenging time constraints representative of an emergency response. Integration of advanced technology environmental sensors will further extend the capability and cost-effectiveness of the envisioned, high-fidelity, fluid dynamics-based forecasting system.

Acknowledgments

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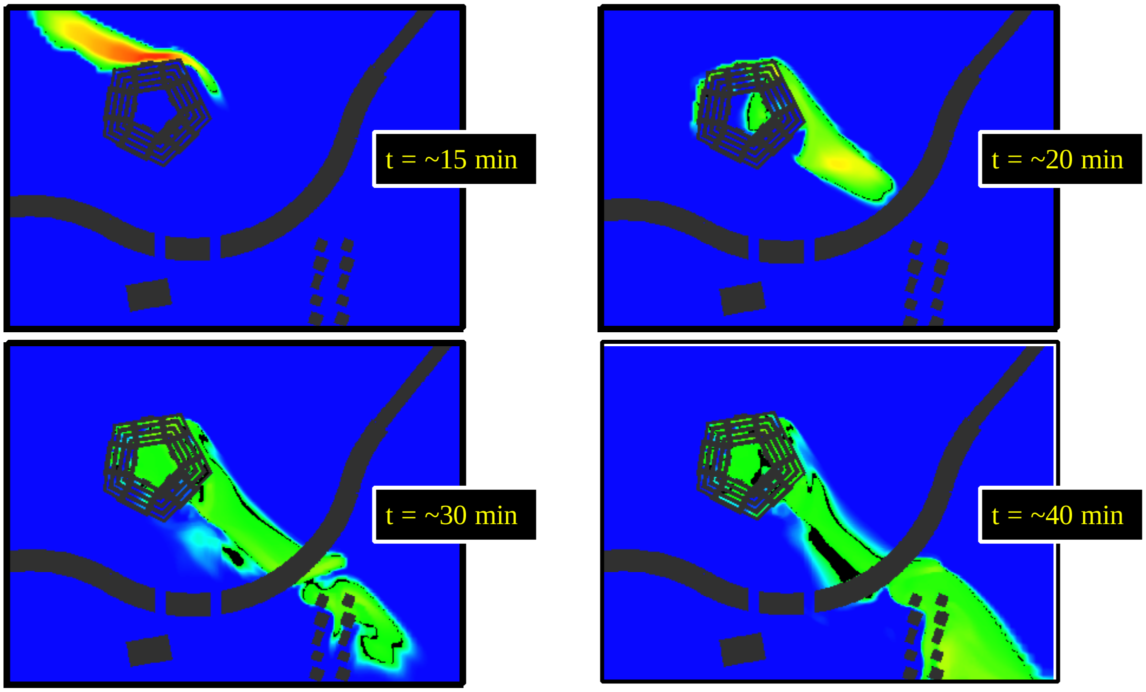

Figure 1. Gas cloud flowing over Pentagon and into Crystal City (1996 computation).

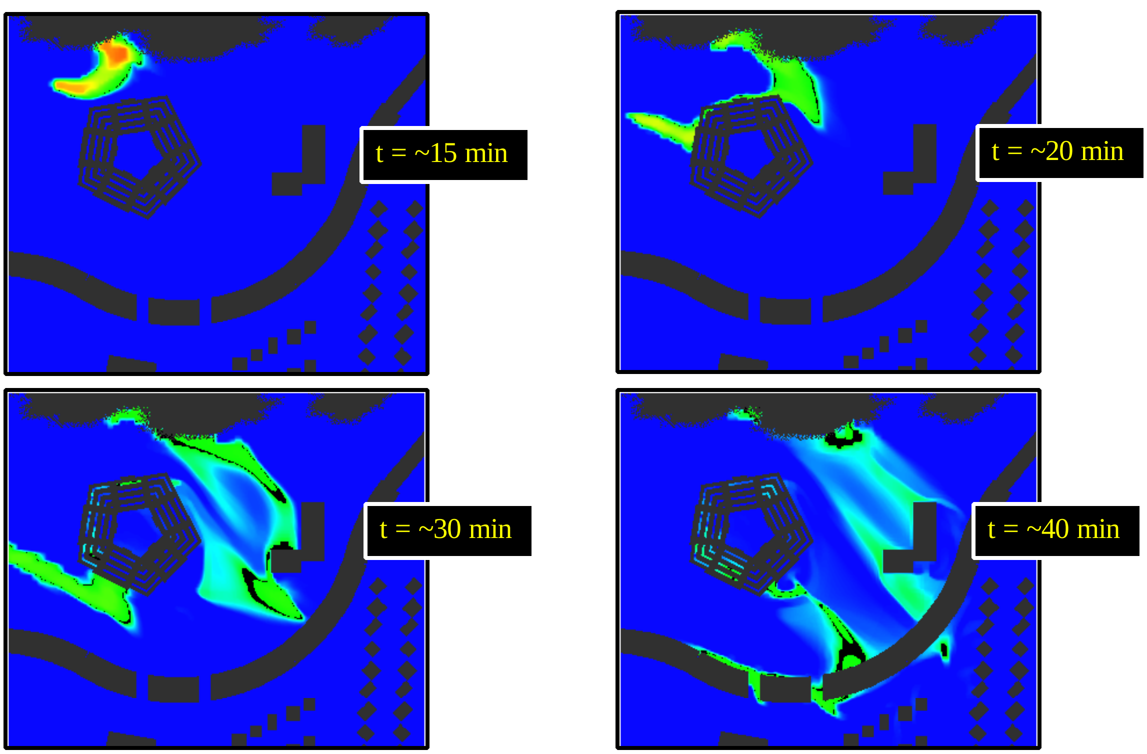

Figure 2. Gas cloud flowing over Pentagon and into Crystal City (1998 computation).

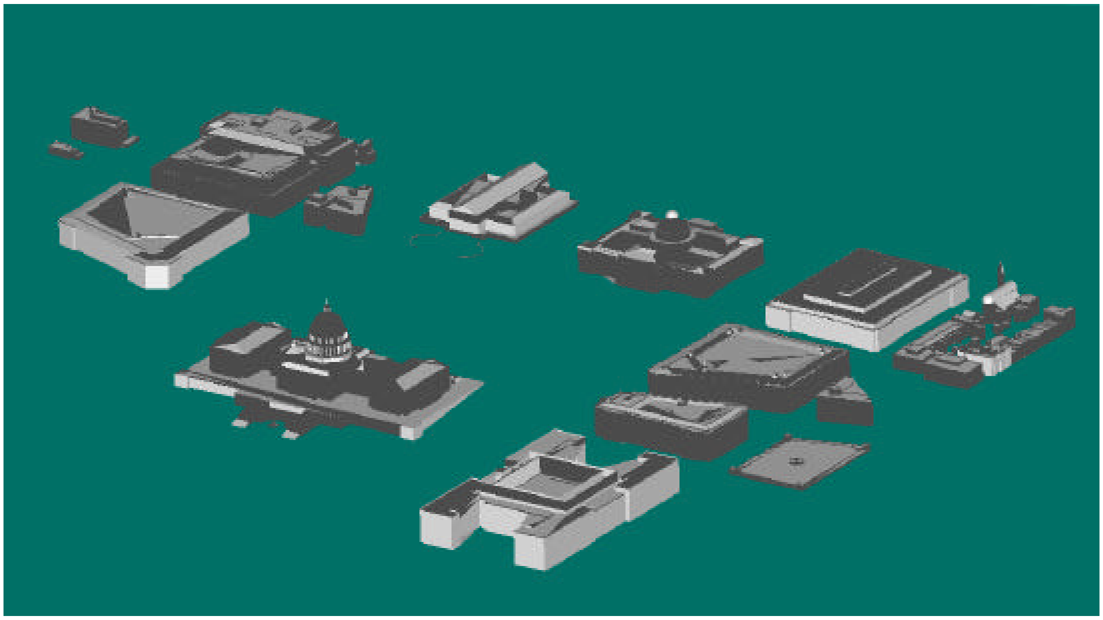

Figure 3. Building portion of geometric database for DC Mall area.

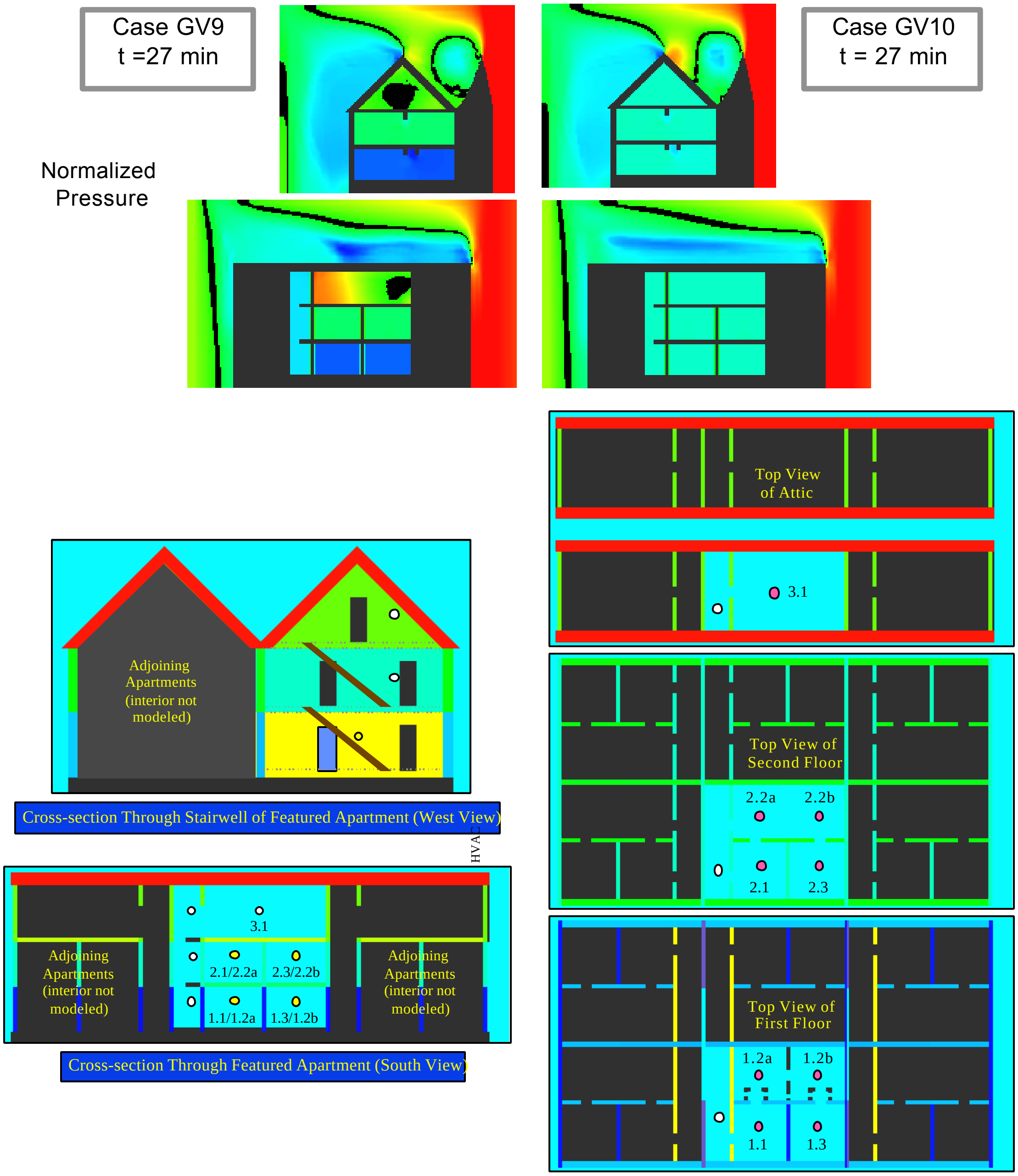

Figure 4. Cross-sectional views of FAST3D-CT apartment definition showing room nomenclature and sampler locations (circles).

Propylene Concentration

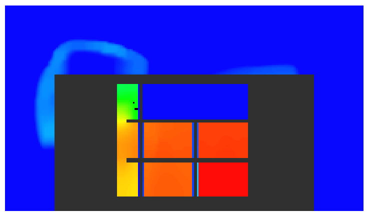

Figure 5: Pressure and propylene distributions predicted by FAST3D-CT at t=27 minutes for Cases GV9 (stairwell door to attic closed) and GV10 (stairwell door to attic open).

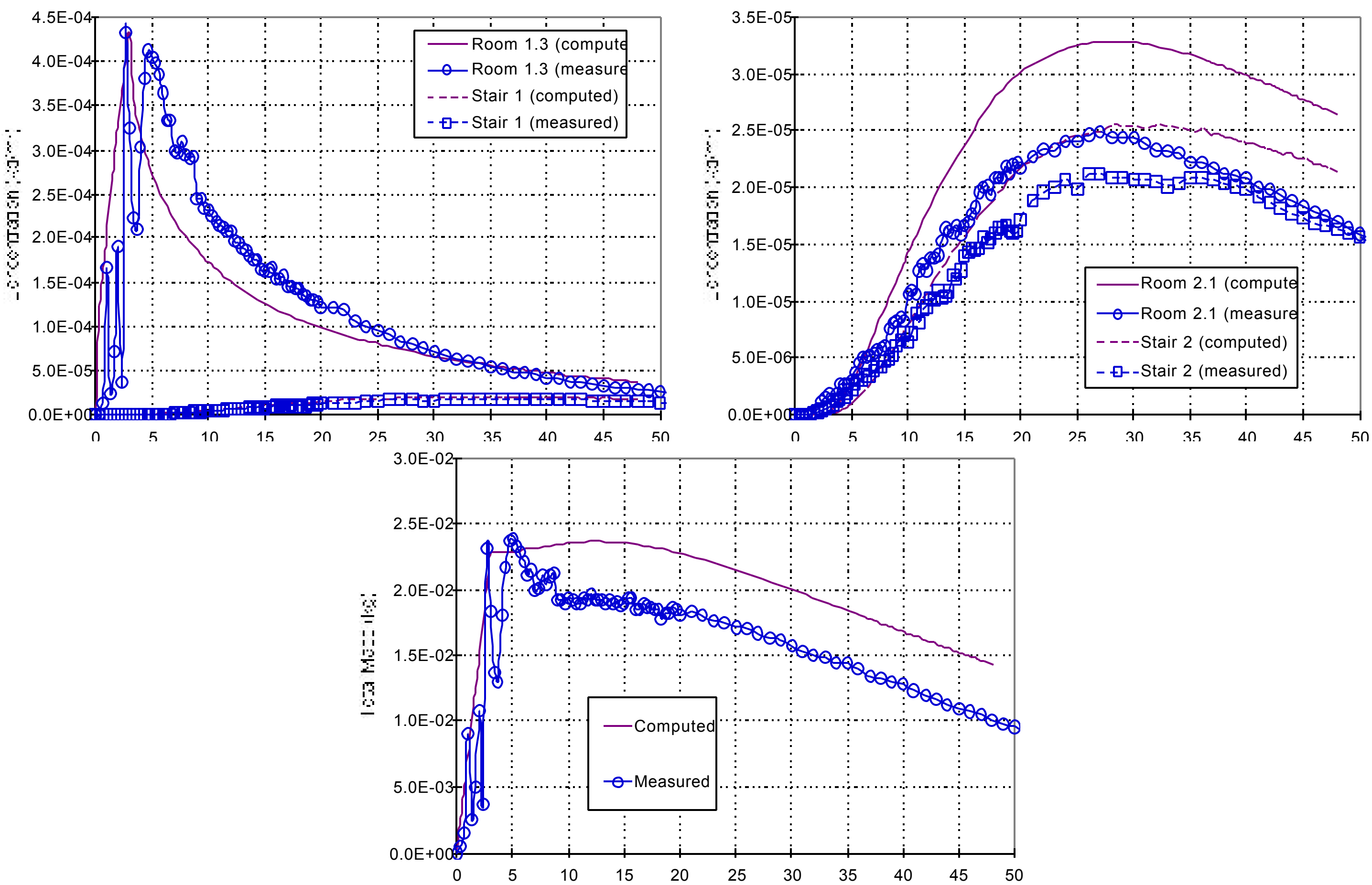

Figure 6. Time histories of propylene concentrations in first-floor (a) and second-floor (b) rooms, and time histories of total propylene in apartment complex (c), run GV9.